

M05.0D 30 Years of Rietveld Refinement

Chair: R. Hill

Co-Chair: A.W. Hewat

Attendance: 200



100 people queuing outside the lecture theatre, unable to get in. Of course they had all come to hear Hugo Rietveld, inventor of the famous Rietveld Refinement that has so revolutionised powder diffraction. Hugo outlined the origins of the method named after him, from his early days at the University of Western Australia to his later work at the Netherlands Energy Research Foundation ECN in Petten on the neutron structures of uranium compounds and other heavy metal ceramics.

Alan Hewat took up the neutron story showing how primitive the original diffractometers were, even at the new European High Flux Reactor (ILL). Today's instruments are very different, with large position sensitive detectors used to collect all available neutrons. Powder diffraction, has had more impact than most other neutron technique, from the study of charge reservoirs in oxide superconductors, to the structure of giant magneto-resistive ceramics.

Fujio Izumi showed how incommensurable structures could be refined, and described a new computer program, REMEDY combining Rietveld and Maximum Entropy techniques to increase real space resolution. He gave examples of complex spin-ladder oxide superconductors, and other inorganic materials among the hot topics in physics today.

Daniel Louer then reported how laboratory X-rays have made a big contribution with automatic indexing and structure solution from powders, transforming the study of solid state chemistry for some materials.

Finally Andy Fitch demonstrated how the very high intensity of synchrotron radiation meant that resolution could be increased to obtain the very precise line positions needed for automatic indexing, and to identify precise crystal symmetry and superstructure. Synchrotron radiation has then become a very powerful technique for the almost automatic solution of unknown structures from very small quantities of powder, and an ideal complement to neutron Rietveld refinement.

Alan Hewat